EXCITON IN QUANTUM TUBE WITH HEXAGON CROSS*

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It is established the theory of exciton spectrum in semiconductor quantum nanotube with hexagon cross in the framework of the effective mass approximation and rectangular potentials model. The electron-hole interaction is taken into account within Bethe method together with the approximating potential providing the bound state of exciton at its internal movement along the axial axis of nanosystem. The dependences of exciton energy on the geometrical parameters of quantum nanotube are analyzed.

Key words: quantum tube, exciton, energy spectrum.

1. INTRODUCTION

The technique of semiconductor quantum size nanoheterosystems production is improved so rapidly that there is the experimental ability to create nanostructures (quantum dots, wires and films) with correct geometrical shape. The perspective of utilization of such quantum nanoobjects in modern electronics, optoelectronics and biomedical electronics is evident and analyzed in details in the observing papers [1–4]. So, for example, the semiconductor nanowires produced from Si, Ge, GaP, GaAs and InP can be used for the creation of logical schemes, super thin light emitting diodes and low dimensional photo detectors.

The theoretical investigation of the above-mentioned systems is rapidly developing but for the multi component nanosystems it is only at the first stage due to their physical phenomena, rather complicated and sophisticated for the mathematical description.

Recently, in ref. [5], it was experimentally investigated the spectrum of luminescent hexagon super lattice, created by InP/InAs/InP nanotubes with the transversal cross-section of right hexagon shape (Fig. 3.1.a). These nanotubes were grown using the metal organic epitaxy method. The geometric parameters of the

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system are taken in such a way that the height of nanotubes (L) is hundreds times bigger than their transversal sizes (b). Since, such nanosystem can be assumed as a super lattice of quantum tubes with infinite height. All nanotubes can be considered as isolated of each other because the lattice constant (a) is much bigger than the transversal size (b) for the individual quantum tube. Therefore, the problem of electron and hole energy spectrum is solved for the single hexagon tube.

2. THEORY OF ELECTRON ENERGY SPECTRUM IN QUANTUM NANOTUBE WITH HEXAGON CROSS

The quantum nanotube of infinite height with transversal hexagon cross (Fig. 1a) is observed. The composition materials of inner cylinder (0), tube (1) and outer medium (2) are assumed as different. The sizes of outer (b) and inner (d) hexagons are fixed, therefore the thickness of semiconductor nanoshell creating the quantum well for the electron is also known: $\Delta = (b-d)/2$. The further analytical calculations are performed for the electron because the theory of electron and hole spectra is qualitatively equal.

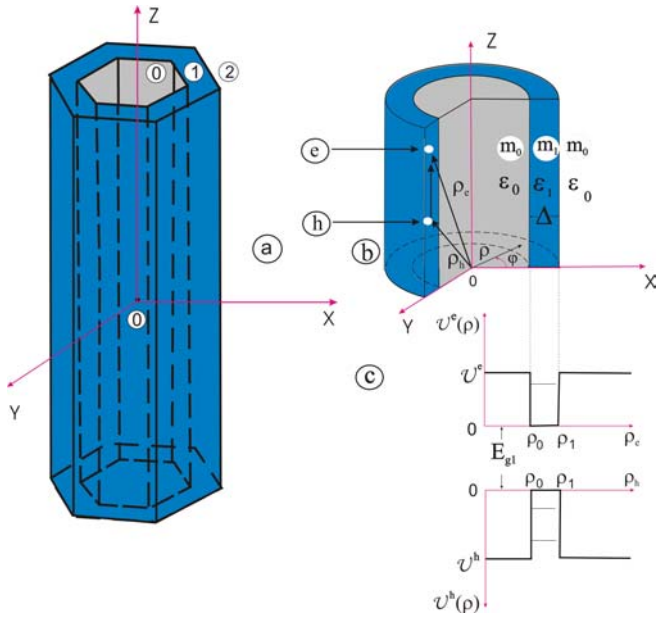

Fig. 1. – Geometrical scheme of hexagon (a) and approximating (b) nanotube and schemes of potential energies (c) of electron and hole in nanosystem.

Energy spectrum and wave functions of electron are defined as the solutions of stationary Schrödinger equation, which in the cylindrical coordinate system has the form

$$\left[-\frac{\hbar^2}{2}\left(\vec{\nabla}_{\rho\varphi}\frac{1}{\mu(\rho,\varphi)}\vec{\nabla}_{\rho\varphi}+\frac{1}{\mu(\rho,\varphi)}\frac{\partial^2}{\partial z^2}\right)+U(\rho,\varphi)\right]\psi(\rho,\varphi,z)=E\psi(\rho,\varphi,z). \quad (1)$$

Here $\mu(\rho,\varphi)$ – the electron effective mass, considered as constant but different for the different semiconductor media creating the nanoheterosystem under research

$$\mu(\rho,\varphi)=\begin{cases}\mu_0, & \text{medium "0"}\\ \mu_1, & \text{medium "1"}\\ \mu_0, & \text{medium "2"}\end{cases}. \quad (2)$$

Since the lattice constants of semiconductor parts of nanoheterosystem have the close magnitudes, the electron potential energy can be written as

$$U(\rho,\varphi)=\begin{cases}U_0, & \text{medium "0"}\\ U_1, & \text{medium "1"}\\ U_0, & \text{medium "2"}\end{cases}. \quad (3)$$

z-th variable in Schrödinger eq. (1) can be separated when the wave function is chosen in the form

$$\psi(\rho,\varphi,z)=F(\rho,\varphi)\frac{1}{\sqrt{L}}e^{ik_{\|}z}, \quad (4)$$

where $k_{\|}$ – the axial wave vector, L – the magnitude of the effective region of electron movement along Oz axis.

The wave function $F(\rho,\varphi)$ satisfies Schrödinger equation

$$\hat{H}_{k_{\|}}F(\rho,\varphi)=\left\{-\frac{\hbar^2}{2}\left(\vec{\nabla}_{\rho\varphi}\frac{1}{\mu(\rho,\varphi)}\vec{\nabla}_{\rho\varphi}+\frac{k_{\|}^2}{\mu(\rho,\varphi)}\right)+U(\rho,\varphi)\right\}F(\rho,\varphi)=E\,F(\rho,\varphi). \quad (5)$$

In order to separate ρ and φ variables in eq. (5) with complicated dependences of $\mu(\rho,\varphi)$ (exp. (2)) and $U(\rho,\varphi)$ (exp. (3)), it is further used the modified Bethe variation method, ref. [6]. Herein, the inner and outer hexagons are approximated by the circles (Fig. 1b), the radii of which are ρ_0 and $\rho_1=\rho_0+\Delta$, where ρ_0 plays the role of variation parameter. Therefore, the Hamiltonian $\hat{H}_{k_{\|}}$ is conveniently to write as

$$\hat{H}_{k_{\|}}(\rho,\varphi)=\hat{H}^{(0)}_{k_{\|}}(\rho,\varphi)+\Delta\hat{H}(\rho,\varphi), \quad (6)$$

where

$$\Delta\widehat{H}(\rho,\varphi)=\widehat{H}_{k_{||}}(\rho,\varphi)-\widehat{H}^{(0)}_{k_{||}}(\rho,\varphi)\,. \tag{7}$$

Here

$$\widehat{H}^{(0)}_{k_{||}}(\rho,\varphi)=-\frac{\hbar^2}{2}\left(\vec{\nabla}_{\rho\varphi}\frac{1}{\mu(\rho)}\vec{\nabla}_{\rho\varphi}+\frac{k_{||}^2}{\mu(\rho)}\right)+U(\rho) \tag{8}$$

– the Hamiltonian, describing the electron in cylindrical semiconductor nanotube with inner and outer radii ρ_0 and ρ_1, respectively and the term

$$\Delta\widehat{H}=\frac{\hbar^2}{2}\left(\vec{\nabla}_{\rho\varphi}\left[\frac{1}{\mu(\rho)}-\frac{1}{\mu(\rho,\varphi)}\right]\vec{\nabla}_{\rho\varphi}-k_{||}^2\left[\frac{1}{\mu(\rho)}-\frac{1}{\mu(\rho,\varphi)}\right]\right)+U(\rho,\varphi)-U(\rho) \tag{9}$$

is the correction to the Hamiltonian $\widehat{H}^{(0)}_{k_{||}}(\rho,\varphi)$, further observed as a perturbation.

The Schrödinger equation with basic Hamiltonian (8) is solved exactly. Herein, the wave function of zeroth approximation is obtained in the form

$$F(\rho,\varphi)=\frac{1}{\sqrt{2\pi}}e^{im\varphi}\begin{cases}A^{(0)}_m\,I_m(\chi^{(0)}_m\rho), & 0\le\rho\le\rho_0\\ A^{(1)}_m\,J_m(\chi^{(1)}_m\rho)+B^{(1)}_m\,N_m(\chi^{(1)}_m\rho), & \rho_0\le\rho\le\rho_1\\ B^{(2)}_m\,K_m(\chi^{(0)}_m\rho), & \rho_1\le\rho<\infty\end{cases}, \tag{10}$$

where $J_m(\chi^{(1)}_m\rho)$, $N_m(\chi^{(1)}_m\rho)$ – Bessel functions of the whole order, $I_m(\chi^{(0)}_m\rho)$, $K_m(\chi^{(0)}_m\rho)$ – modified Bessel functions, $\chi^{(0)}_m=\sqrt{\frac{2\mu_0(U-E)}{\hbar^2}+k_{||}^2}$, $\chi^{(1)}_m=\sqrt{\frac{2\mu_1 E}{\hbar^2}-k_{||}^2}$, $U=U_1-U_0$, m – magnetic quantum number.

The conditions of wave functions and densities of probability currents continuity in points $\rho=\rho_0$ and $\rho=\rho_0+\Delta$ together with the normalizing condition determine all unknown coefficients A_m, B_m in exp. (10). Thus, the wave function $F^{(0)}_{nm}(\rho,\varphi)$ is fixed and dispersion equation is defining the electron energy $E^{(0)}_{nm}(k_{||},\rho_0)$ (quantum number n numerates the solutions of dispersion equation at the fixed magnitudes of magnetic quantum number m).

Corrections $\Delta E_{nm}(k_{||},\rho_0)$ to the energy $E^{(0)}_{nm}(k_{||},\rho_0)$, according to the Bethe method, are further obtained as diagonal matrix elements of operator $\Delta\widehat{H}(\rho,\varphi)$ (9) at the functions (10)

$$\Delta E_{n\,m}(k_{\|},\rho_0)=\left\langle nm\left|\Delta\hat{H}(\rho,\,\varphi)\right|nm\right\rangle. \qquad (11)$$

Finding the magnitude $\rho_0^{n\,m}$, realizing minimum of the electron energy $E_{n\,m}(k_{\|},\rho_0)=E_{nm}^{(0)}(k_{\|},\rho_0)+\Delta E_{n\,m}(k_{\|},\rho_0)$, one can obtain the electron spectrum in quantum nanotube with hexagon cross

$$E_{n\,m}^{(e)}(k_{\|},\rho_0^{n\,m})=E_{nm}^{(0)(e)}(k_{\|},\rho_0^{n\,m})+\Delta E_{n\,m}^{(e)}(k_{\|},\rho_0^{n\,m}). \qquad (12)$$

The analogical considerations bring to the hole energy spectrum $E_{n\,m}^{(h)}(k_{\|},\rho_0^{n\,m})$ and its wave functions $F_{n\,m}^{(0)\,(h)}$.

3. EXCITON SPECTRUM IN HEXAGON NANOTUBE

In the space of nanotube, where the electron is mainly moving, the Hamiltonian of interacting electron and hole in the system of mass center over z_e and z_h variables and taking into account the forbidden band width (E_{g1}) of nanotube medium, is written as

$$\hat{H}=-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial Z^2}-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2}-\frac{e^2}{\varepsilon_1}\frac{1}{\sqrt{z^2+(\vec{\rho}_e-\vec{\rho}_h)^2}}+\hat{H}_{k_{\|}}^{e}(\rho,\varphi)+\hat{H}_{k_{\|}}^{h}(\rho,\varphi), \qquad (13)$$

where $M=\mu_1^e+\mu_1^h$, $\mu=\dfrac{\mu_1^e\,\mu_1^h}{\mu_1^e+\mu_1^h}$ – the effective mass of exciton longitudinal movement, as a whole and reduced mass of electron and hole movement along Oz axis, respectively; ε_1 – dielectric constant of nanotube medium; $Z=\dfrac{\mu_1^e z_e+\mu_1^h z_h}{\mu_1^e+\mu_1^h}$; $z=z_e-z_h$.

As one can see from exp. (13), the movement of exciton mass center along OZ axis is separated and the energy E_P and wave function $\psi_P(Z)$ of exciton longitudinal movement are the following

$$E_P=\frac{P^2}{2M},\qquad \psi_P(Z)=\frac{1}{\sqrt{2\pi\hbar}}e^{iPZ/\hbar}. \qquad (14)$$

Further, according to the Bethe method (ref. [6]), in the Hamiltonian (13) it is added and subtracted the potential

$$U(z) = -\frac{V_0}{ch^2(z/a)}, \qquad V_0 = \frac{e^2}{\varepsilon_1 a} \tag{15}$$

with variation parameter a. Such potential together with z-th kinetic energy component gives the energy of bound state ($E_n^{(0)}$) and, on the other hand, in the subtraction with the potential of electron-hole interaction, it forms a small magnitude in the sense of perturbation theory

$$\Delta U = \frac{V_0}{ch^2(z/a)} - \frac{e^2}{\varepsilon_1\sqrt{z^2 + (\rho_e - \rho_h)^2 + 4\rho_e\rho_h \sin^2(\varphi_e - \varphi_h)}}. \tag{16}$$

The Schrödinger equation with Hamiltonian

$$\hat{H}_{\|} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} - \frac{V_0}{ch^2(z/a)} \tag{17}$$

has the exact solution, ref. [7]

$$\begin{gathered} E_n^{(0)} = -\hbar^2\varepsilon_n^2 / 2\mu a^2, \\ \psi_n(\xi) = (1-\xi^2)^{\varepsilon_n/2}\, F(\varepsilon_n - S,\ \varepsilon_n + S + 1,\ \varepsilon_n + 1,\ (1-\xi)/2) \end{gathered}, \tag{18}$$

where $\varepsilon_n = 2S - (1/2 + 2n)$, $S = 1\Big/2\left(\sqrt{1 + \frac{8\mu a}{\varepsilon_1 m_0 a_B}} + 1\right)$, $n = 0, 1, 2, \ldots$, $\xi = \mathrm{th}(z/a)$.

Thus, the exciton energy and wave functions depend on the variation parameter (a) and are fixed by the expressions

$$E_{n_h m_h}^{n_e m_e}(n, a, P) = E_{n_e m_e} + E_{n_h m_h} + E_{g1} + \frac{P^2}{2M} + \Delta E_{n_h m_h}^{n_e m_e}(n, a), \tag{19}$$

$$\psi_{n_h m_h}^{n_e m_e}(n, a, P) = \psi_P(Z)\,\psi_n(a, z)\,\psi_{n_e m_e}(\rho_e, \varphi_e)\,\psi_{n_h m_h}(\rho_h, \varphi_h) = \left| \begin{matrix} n_e & m_e \\ n_h & m_h \end{matrix} n\, P \right>, \tag{20}$$

$$\Delta E_{n_h m_h}^{n_e m_e}(n, a) = \left< \begin{matrix} n_e & m_e \\ n_h & m_h \end{matrix} n\, P \left| \Delta U \right| \begin{matrix} n_e & m_e \\ n_h & m_h \end{matrix} n\, P \right>. \tag{21}$$

The final magnitude of the exciton energy is obtained after the minimization of exp. (19) over the variation parameter a.

4. DISCUSSION OF THE RESULTS

The computer calculations of exciton energy spectrum in hexagon nanotube have been performed for the nanosystem InP/InAs/InP, described and experimentally investigated in ref. [5].

In Fig. 2a, b, c it is shown the dependence of electron transversal movement energy: $E^{e}_{n,m}$ (a), electron and hole binding energy: ΔE^{10}_{10} (b) and energy of ground exciton state: E^{10}_{10} (c) on the nanotube inner radius ρ_0 at its different thicknesses Δ. From the figure one can see the main properties of the spectrum:

1. The variation of inner nanotube radius (ρ_0), independently on Δ magnitude brings to the variation of the location of electron energy level in energy scale respectively the one, it has in the quantum wire with radius Δ till the one, it has in the plane film with the thickness Δ. It is clear from the physical considerations.
2. The evolution of the electron spectrum for the small $(\Delta \le 10\text{nm})$ and big $(\Delta > 10\text{nm})$ magnitudes of Δ is quite different due to the fact that at the increasing of the well width Δ (equal for the nanotube and quantum film) the ground levels in nanotube and quantum film are decreasing with different velocity (it is seen at the figure).
3. At the decreasing of ρ_0 magnitude the ground electron energy levels are shifting into the region of smaller energies and, or passing the minimum, are further reaching the ground levels in quantum wire with radius Δ if they are located over the levels in quantum film, or this minimum is approached at $\rho_0 \to 0$, if the level in quantum wire is located lower the level in quantum film.

It is to be mentioned that the behavior of the hole energy spectra is qualitatively similar to the electron one and the quantitative difference is caused only by the difference of effective masses and potential energies of quasiparticles.

In Fig. 2b it is presented the dependence of exciton binding energy on the magnitude of nanotube inner radius (ρ_0) at different values of its thickness Δ. Figure proves that the decreasing of ρ_0 at $\Delta = \text{const}$ brings to the increasing of exciton binding energy, due to the bigger region for its spatial localization. The absolute magnitude of exciton binding energy for the nanotube with the thickness 1–5nm is two orders smaller than the electron or hole energy $E^{e,h}_{10}$. Therefore, the dependence of ground state exciton energy (E^{10}_{10}) on nanotube geometrical parameters is mainly caused by the peculiarities of the behavior of electron and hole ground energy states, as it is seen at the Fig. 2c.

Fig. 2c proves that the theoretically calculated magnitude of exciton energy in nanotube with the thickness $\Delta = 1.5 \div 2.5\text{nm}$ well correlates to the experimental (ref. [5]) location of the pick in energy scale ($E_{\exp} \sim 860meV \pm 40meV$). The future more exact theoretical accounting of nanotube geometric characteristics, electron- and exciton-phonon interaction and interaction with impurities and also the improvement of experimental abilities for the creation of homogenous nanotubes

(especially over the sizes) provides the hope for the well correlation between the theory and experiment.

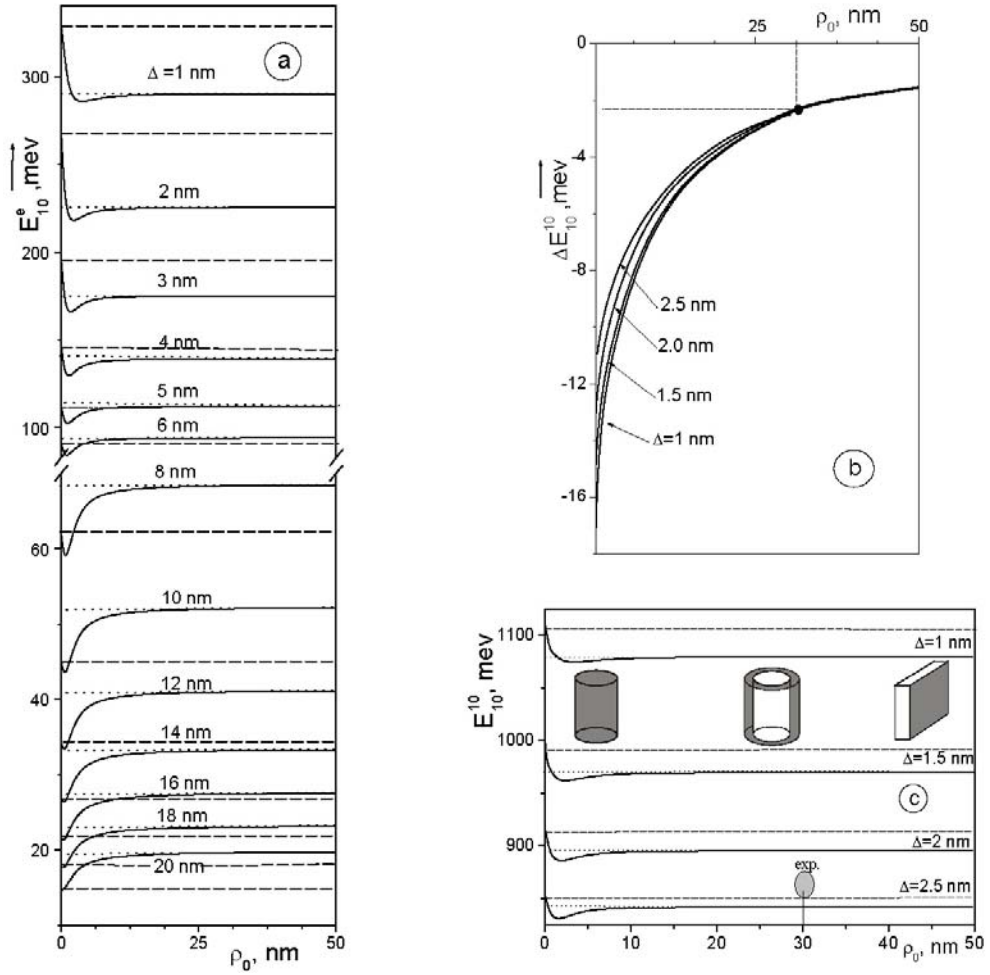

Fig. 2. – Dependence of electron transversal movement energy (a), electron-hole binding energy (b) and ground state exciton energy (c) on the inner nanotube radius ρ_0 at its different thicknesses Δ.

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